

Maximal core size in singular graphs

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Abstract

A graph G is singular of nullity η if the nullspace of its adjacency matrix \mathbf{G} has dimension η . Such a graph contains η cores determined by a basis for the nullspace of \mathbf{G} . These are induced subgraphs of singular configurations, the latter occurring as induced subgraphs of G . We show that there exists a set of η distinct vertices representing the singular configurations. We also explore how the nullity controls the size of the singular substructures and characterize those graphs of maximal nullity containing a substructure reaching maximal size.

Keywords: Adjacency matrix, nullity, extremal singular graphs, singular configurations, core width.

Math. Subj. Class.: 05C50, 05C60, 05B20.

1 Introduction

A graph $G = G(\mathcal{V}, \mathcal{E})$ has vertex set $\mathcal{V} = \mathcal{V}_G = \{1, 2, \dots, n\}$ and edge set \mathcal{E} consisting of pairs of vertices. The *order* $|G|$ of a graph G is the number n of vertices. The graphs we consider are simple, that is, without multiple edges or loops. The complete graph K_n on n vertices has edges between all distinct pairs of vertices.

The graph $G - X$ denotes the graph obtained from G when the set X of vertices and the edges incident to the vertices in X are deleted. The reverse process, starting from H and adding a vertex set X results in $H + X$. Note that $H + X$ is not unique for a particular graph H and set X , since it varies with the choice of edges between X and \mathcal{V}_H and even with the edges among the vertices of X themselves. If $X = \{v\}$, we write $G - v$ and $G + v$ for $G - X$ and $G + X$ respectively.

The adjacency matrix of a graph G , denoted by \mathbf{G} , is (a_{ij}) , where $a_{ij} = 1$ if $\{ij\}$ is an edge and 0 otherwise. Note that the set of matrices $\{\mathbf{G}\}$ for distinct labellings of the vertices are permutationally similar and therefore a graph G is described completely (up

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to isomorphism) by the corresponding \mathbf{G} for a specific labelling. The *spectrum* $Sp(G)$ of a graph G consists of the collection, with repetitions, of the eigenvalues of \mathbf{G} , which are the solutions of the characteristic equation $\det(\lambda\mathbf{I} - \mathbf{G}) = 0$. The *algebraic multiplicity* of an eigenvalue is the number of times it is repeated in $Sp(G)$. The *geometric multiplicity* is the dimension of the corresponding eigenspace. Since \mathbf{G} is real and symmetric, the two multiplicities for an eigenvalue have a common value. The multiplicity of the eigenvalue zero is referred to as the *nullity*¹, $\eta(G)$, of G . The *rank* of G is $\text{rank}(\mathbf{G})$, equal to $n - \eta(G)$, a result referred to as *the Dimension Theorem*.

A graph G on n vertices is said to be *singular* if $\eta(G) > 0$; that is, if there exists $\mathbf{x} \neq \mathbf{0}$, $\mathbf{x} \in \mathbb{R}^n$, such that $\mathbf{G}\mathbf{x} = \mathbf{0}$, where each entry of the vector $\mathbf{0}$ is 0. Since \mathbf{G} satisfies $\mathbf{G}\mathbf{x} = \lambda\mathbf{x}$ for the eigenvalue $\lambda = 0$, we call \mathbf{x} a *kernel eigenvector* of G .

This paper is motivated by the question:

How does the nullity control the size of the singular substructures within a graph?

This we address in section 4. To this end, we survey results on substructures in section 2 and on certain invariants of a graph in section 3, including proofs of theorems that facilitate the reasoning of new results, leading to a clarification of the underlying concepts.

2 Singular graphs

Let $\mathbf{x} \in \mathbb{R}^n$, $n \geq 3$, be a vector in the nullspace of G , which is labelled so that $\mathbf{x} = (\mathbf{x}_F, \mathbf{0})^t$, with each entry of \mathbf{x}_F being non-zero. The vertices corresponding to \mathbf{x}_F induce a subgraph F whose adjacency matrix is the principal $|F| \times |F|$ submatrix \mathbf{F} of \mathbf{G} , satisfying $\mathbf{F}\mathbf{x}_F = \mathbf{0}$. We call (F, \mathbf{x}_F) , or simply F , a *core of G* . If $\mathbf{x} = \mathbf{x}_F$, then $G = F$ and G is said to be a *core graph*. Note that a core of G is a core graph in its own right. Linearly independent kernel eigenvectors determine distinct cores of G . The set CV of *core vertices* consists of those vertices that lie on some core of G . If a vertex does not lie on any core of G , then it is said to be *core forbidden*. A core graph without isolated vertices having nullity one must be connected and is said to be a *nut graph*. Nut graphs exist for all orders from seven onwards. There are three nut graphs of order seven and none for smaller order [10].

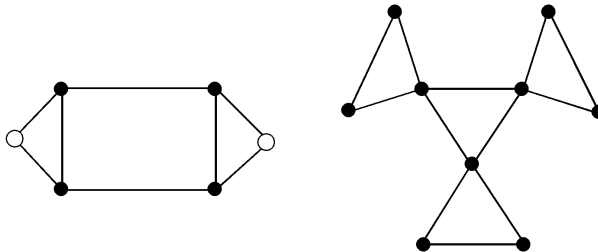


Figure 1: Two singular graphs of nullity one.

Consider the two graphs in Figure 1. The six vertex graph has a nullvector $(1, 1, -1, -1, 0, 0)^t$ and its core is the four cycle C_4 (labelled 1,2,3,4), induced by the solid black vertices, while its core-forbidden vertices (labelled 5,6) are white. The nine vertex graph is a nut graph and therefore has no core-forbidden vertices.

¹The term **corank**(\mathbf{G}) is also used for nullity(\mathbf{G}) in the literature.

Since it is the existence of $\mathbf{x}_F \in \mathbb{R}^{|F|}$ that determines that a graph is singular, we classify singular graphs according to core-order $|F|$. As shown in Figure 2, there are eight possible cores of order six, three of order five, two of order four and one each of orders three and two.


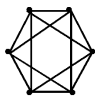

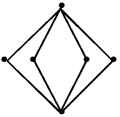

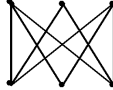

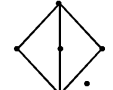

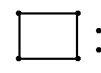
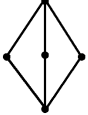



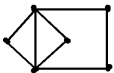
τ	Min-Max Core	Min-rk	τ	Min-Max Core	Min-rk
2		2	6		7
3		4	6		8
4		4	6		8
4		6	6		8
5		6	6		8
5		6	6		10
5		8	7		6 to 12
6		6	$n > 7$		$n-1$ to $2n-2$
6		6			

Figure 2: Minimum rank of graphs with core-width τ .

2.1 Singular configurations

Cauchy’s inequalities for a Hermitian matrix M , (also known as the *Interlacing Theorem* [3]) control the multiplicity of the eigenvalues of principal submatrices relative to those of M . Applied to graphs we have:

Theorem 2.1. *Interlacing Theorem: Let G be an n -vertex graph and $v \in \mathcal{V}$. If the eigenvalues of G are $\lambda_1, \lambda_2, \dots, \lambda_n$ and those of $G-v$ are $\mu_1, \mu_2, \dots, \mu_{n-1}$, both in non-increasing order of magnitude, then $\lambda_1 \geq \mu_1 \geq \lambda_2 \geq \mu_2 \geq \dots \geq \mu_{n-1} \geq \lambda_n$.*

Thus when a vertex is added to a graph, the nullity, or multiplicity of the eigenvalue zero, may change by at most one. Let us first consider a graph of nullity one. Such a graph G with nullspace generator \mathbf{x} has a unique core F as an induced subgraph determined by the vertices corresponding to the non-zero restriction \mathbf{x}_F of \mathbf{x} . We say the core is (F, \mathbf{x}_F) when \mathbf{x}_F needs to be emphasized. By interlacing, to obtain a graph G of nullity one from a core graph F of nullity η , at least $\eta - 1$ vertices are added. Thus a lower bound for the order of a graph G of nullity one, with core (F, \mathbf{x}_F) , is $|F| + \eta(F) - 1$.

Definition 2.2. A graph G , $|G| \geq 3$, is a **singular configuration (SC)**, with core (F, \mathbf{x}_F) , if it is a singular graph, of nullity one, having $|F| + \eta(F) - 1$ vertices, with F as an induced subgraph, satisfying $|F| \geq 2$, $\mathbf{F}\mathbf{x}_F = \mathbf{0}$ and $\mathbf{G} \begin{pmatrix} \mathbf{x}_F \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}$. The vector \mathbf{x}_F is said to be the **non-zero part** of the kernel eigenvector $\begin{pmatrix} \mathbf{x}_F \\ \mathbf{0} \end{pmatrix}$ of G .

Note that by interlacing, among singular graphs of nullity one, a singular configuration G has the least number of vertices for its core (F, \mathbf{x}_F) . A core graph may be connected as in the cycles C_{4k} , $k \in \mathbb{Z}^+$ on $4k$ vertices or disconnected as in the empty graph rK_1 consisting of r isolated vertices. An important combinatorial property of core graphs is that they have no pendant edges.

Lemma 2.3. *A singular configuration is a connected graph.*

Proof. Suppose, for contradiction that a singular configuration S is disconnected. Without loss of generality, S has a connected component S_1 , $|S_1| \geq 3$, having a non-zero kernel eigenvector \mathbf{x}_1 . If the vertices of S_1 are labelled first, then $\mathbf{S} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}$ and $\mathbf{S}_1\mathbf{x}_1 = \mathbf{0}$. Note that S cannot have isolated vertices, since these would contribute to the nullity, so that $\eta(S)$ would be more than one. Since $\mathbf{x}_1 \neq \mathbf{0}$, then $\mathbf{x}_2 = \mathbf{0}$, otherwise $\begin{pmatrix} \mathbf{x}_1 \\ \mathbf{0} \end{pmatrix}$ and $\begin{pmatrix} \mathbf{0} \\ \mathbf{x}_2 \end{pmatrix}$ would be linearly independent kernel eigenvectors of S , again contradicting that the nullity of S is one. Thus the unique core of S lies in S_1 . Suppose that \mathbf{x}_2 corresponds to vertices in the non-singular components. But then S does not have a minimum number of vertices for core F , a contradiction. Thus $S = S_1$. \square

We now show the relevance of singular configurations. We prove that for nullity–one graphs, of order larger than minimal with respect to core F , some singular configuration is an induced subgraph.

Proposition 2.4. *A graph G without isolated vertices, of nullity one, with core (F, \mathbf{x}_F) , has (at least) one induced subgraph which is a singular configuration with the same core (F, \mathbf{x}_F) .*

Proof. Let the vertices of F be labelled first. Then the first $|F|$ rows of \mathbf{G} may be partitioned as $(\mathbf{F}|\mathbf{C})$ and $(\mathbf{F}|\mathbf{C})^t(\mathbf{x}_F) = 0$. Moreover the rank of $(\mathbf{F}|\mathbf{C})$ is $|F| - 1$. If F is not itself a SC, its nullity $\eta(F)$ is more than one. There exist $\eta(F) - 1$ column vectors of the supplementary matrix \mathbf{C} which are mutually linearly independent and also independent of the columns of F . These form the matrix \mathbf{C}' such that $\text{rank}((\mathbf{F}|\mathbf{C}')) = \text{rank}((\mathbf{F}|\mathbf{C})) = |F| - 1$. The principal submatrix of $\mathbf{A}(G)$ determined by $(\mathbf{A}(F)|\mathbf{C}')$ is of the form $\mathbf{A}' = \begin{pmatrix} \mathbf{A}(F) & \mathbf{C}' \\ (\mathbf{C}')^t & \mathbf{Q} \end{pmatrix}$, where \mathbf{Q} is a square matrix. The adjacency matrix \mathbf{A}' defines an induced subgraph of G , satisfying Definition 2.2. Therefore G is a singular configuration $S(F, \mathbf{x}_F)$. \square

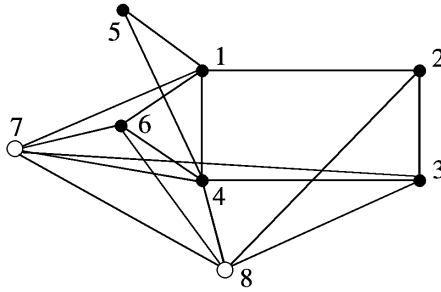


Figure 3: Vertices 7 and 8 are core–forbidden.

Example 2.5. A singular configuration S has a unique core (F, \mathbf{x}_F) whose vertices form the full set \mathcal{CV} in S . If the set \mathcal{P} of core-forbidden² vertices form an independent subset of the vertices of S , then S is said to be a *minimal configuration*. In fact there are $2^{|\mathcal{P}|}$ singular configurations $\{S\}$ obtained from a particular minimal configuration by adding edges between some pairs of distinct vertices of \mathcal{P} and they all satisfy $\mathbf{S} \begin{pmatrix} \mathbf{x}_F \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}$.

The complete list of minimal configurations of core order up to five may be found in [5].

The singular graph G , of nullity one, shown in Figure 3, has only one core F which is the subgraph (of order 6 and nullity 2) induced by the solid black vertices. By Definition 2.2, a singular configuration with core F is expected to have 7 vertices. There are two non-isomorphic singular configurations, $G - 7$ and $G - 8$, having the same core as G . These two distinct induced subgraphs of G are in fact minimal configurations. Moreover, G and its two singular configurations share the same non-zero part $\mathbf{x}_F = (1, 1, -1, -1, -1, 1)^t$ of a kernel eigenvector generating their nullspace.

3 Some new invariants of singular graphs

The study of singular graphs reveals invariants of a graph. One is the partition of the vertex set $\mathcal{V}(G)$ into the set \mathcal{CV} of vertices lying on some core of G and the set of core-forbidden vertices, $\mathcal{V}(G) \setminus \mathcal{CV}$. We show that this partition does not depend on the choice of basis for the nullspace of \mathbf{G} . Therefore \mathcal{CV} is well defined.

Proposition 3.1. *The set \mathcal{CV} of core vertices is an invariant of a graph G .*

Proof. A basis B for the nullspace can be transformed into another, B' , by linear combinations of the vectors of B . However, the union of the collections of the positions of the non-zero entries in the basis vectors is the same for all bases. Thus the partition of the vertex set $\mathcal{V}(G)$ into \mathcal{CV} and core-forbidden vertices, $\mathcal{V}(G) \setminus \mathcal{CV}$, is independent of the basis used for the nullspace. \square

²For a graph G of nullity more than one, the *periphery* with respect to F is the subset of vertices *not* on the core F . For graphs of nullity more than one, the set of core-forbidden vertices is then the set–intersection of the peripheries over all cores F of G .

From proposition 3.1, it follows that the set, $\mathcal{V}(G) \setminus CV$, of core-forbidden vertices is also an invariant of G .

3.1 Fundamental system of cores

We now point out properties of subspaces in general that shed light on the structure of a singular graph. For any vector space W , let $wt(\mathbf{x})$ denote the **weight** or number of non-zero entries of the vector \mathbf{x} . We adopt the convention to write a basis for a vector space in which the vectors are *ordered* according to the monotonic non-decreasing *sequence* of the weights of its vectors.

A maximal set of linearly independent vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_\ell$, with the smallest *weight sum* $\sum_{i=1}^\ell wt(\mathbf{x}_i)$, are said to form a *minimal basis* B_{min} for W . We say a basis B for W is *reducible* if linear combinations of the vectors of B can produce another basis for W with lower weight sum. Thus for any vector space, a basis is not reducible if and only if it is minimal. The monotonic non-decreasing sequence of weights of vectors (weight–sequence) in a minimal basis provides an invariant of the vector space, a result that is significant because of its generality to bases of any vector space:

Theorem 3.2. [8] *Let W be a q –dimensional subspace of \mathbb{R}^n . Let t_1 be the least weight of a non-zero vector in W and let $B_1 = (\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_q)$, with weight–sequence t_1, t_2, \dots, t_q , be a basis with minimum weight-sum. If $B_2 = (\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_q)$ is another ordered basis for W with weight–sequence s_1, s_2, \dots, s_q , then $\forall i, t_i \leq s_i$.*

Although there may be various possible minimal bases for a vector space, by Proposition 3.2, the sequence of weights of their members is unique for the vector space. The following results are immediate.

Corollary 3.3. *A basis for a vector space is not reducible if and only if the monotonic non-decreasing sequence of the weights of its vectors is lexicographically minimal.*

Corollary 3.4. *The weight–sequence of a minimal basis for a vector space is an invariant of the vector space.*

The vertex space for a n -vertex graph G is considered to be \mathbb{R}^n and the nullspace $\ker(\mathbf{G})$, is a subspace of dimension η . Note that a minimal basis B_{min} for $\ker(\mathbf{G})$ determines a *fundamental system of cores* of G . We now apply Corollary 3.4 to singular graphs to obtain another invariant associated with the nullspace.

Proposition 3.5. *The monotonic non–decreasing sequence of core-orders in a fundamental system of cores is a graph invariant.*

Remark 3.6. The following result proved in [7], provides a necessary condition, in terms of admissible subgraphs, for a graph to be of a specific nullity η .

Proposition 3.7. *Let H be a singular graph, without isolated vertices, having nullity η . There exist η SCs as induced subgraphs of H whose cores form a fundamental system of cores of H .*

3.2 Increasing the nullity of a graph

Proposition 3.7 provides a necessary condition for a graph to be of nullity η . The following proposition, which we shall use repeatedly in what follows, gives a necessary and sufficient condition to increase the number of core vertices in a graph.

Proposition 3.8. *The nullity increases with the addition of a vertex v to a graph G forming a connected graph $G + v$ if and only if v is a core vertex of $(G + v)$.*

Proof. Suppose, for contradiction, that v does not lie on any core of the resulting graph $G + v$ but $\eta(G) < \eta(G + v)$. Then all the cores of $G + v$ lie in G . But then, interlacing demands that $\eta(G) \geq \eta(G + v)$, a contradiction.

Conversely, let v be a core vertex of $(G + v)$. Then there exists a kernel eigenvector \mathbf{x} with a non-zero entry corresponding to v . Let \mathbf{M} be the $k \times n$ matrix whose rows are the k vectors of a basis for the nullspace of $G + v$, labelled so that the first row of \mathbf{M} is \mathbf{x} and the first column corresponds to v . By row-reducing \mathbf{M} to echelon form, with all entries in the columns above and below a leading 1 (or pivot) being zero, a matrix \mathbf{M}' is produced, whose rows give a new basis $B_{\mathcal{Y}}$ for the nullspace of $G + v$, determining a system \mathcal{Y} of cores. The first row determines the only core F in this system with vertex v . Deleting v has the effect of destroying F while retaining all the other cores in \mathcal{Y} . Thus $\eta(G) \geq \eta(G + v) - 1$.

Moreover, if $\eta(G) > \eta(G + v) - 1$, then there exists a kernel eigenvector \mathbf{z} of G which is linearly independent of those determined by \mathcal{Y} . This kernel eigenvector becomes an additional kernel eigenvector of $G + v$ by adding a zero as a first entry; but then the $k + 1$ vectors in $B_{\mathcal{Y}} \cup \{\mathbf{z}\}$ are linearly independent in the k -dimensional nullspace of $G + v$, a contradiction. Hence $\eta(G) = \eta(G + v) - 1$. □

We now show that if a graph G of rank r is labelled so that the first r rows of \mathbf{G} are linearly independent, then \mathbf{G} has a simple block form.

Proposition 3.9. *Let the graph G be of order n and rank r , with adjacency matrix \mathbf{G} . Let the first r rows of \mathbf{G} be linearly independent vectors. Then there exist a non-singular $r \times r$ matrix \mathbf{B} and a $r \times (n - r)$ matrix \mathbf{Y} such that*

$$\mathbf{A}(G) = \begin{pmatrix} \mathbf{B} & \mathbf{BY} \\ \mathbf{Y}^t\mathbf{B} & \mathbf{Y}^t\mathbf{BY} \end{pmatrix}.$$

Proof. The first r rows of \mathbf{G} form a submatrix \mathbf{T} of the adjacency matrix \mathbf{G} and represent a maximal set of linearly independent row vectors of \mathbf{G} . Each of the $\eta(G)$ row vectors R_j , $j > r$, is linearly dependent on a subset of the first r row vectors of \mathbf{G} . The adjacency matrix \mathbf{G} , of rank r and nullity η , can be expressed as $\begin{pmatrix} \mathbf{T} \\ \mathbf{Y}^t\mathbf{T} \end{pmatrix}$ for a $r \times \eta$ matrix \mathbf{Y} . To see this, note that each linear relation between R_j , $j > r$ and the rows of \mathbf{T} corresponds to a kernel eigenvector in the nullspace of \mathbf{G} . Since each of these $\eta(G)$ kernel eigenvectors corresponds to a core with a unique vertex v_j (described by row vector R_j , $j > r$), these $\eta(G)$ kernel eigenvectors are linearly independent and so their first r entries form the columns of \mathbf{Y} . Because of the symmetry of \mathbf{G} , the block \mathbf{T} can be expressed as $(\mathbf{B} \ \mathbf{BY})$, where \mathbf{B} is a $r \times r$ non-singular matrix. The result now follows immediately from the symmetry of \mathbf{G} . □

Note that in general there are different choices of the first r rows. Also, each of the last $(n - r)$ vertices in this labelling of G lies on a core and are said to form a **singular configuration vertex-representation** denoted by \mathcal{R} . Thus $|\mathcal{R}| = n - r = \eta$, by the Dimension Theorem. The kernel eigenvectors, forming a basis for the nullspace of \mathbf{G} , define a system \mathcal{Y} of η distinct cores that correspond to η singular configurations found as induced subgraphs of G . There is a one-one correspondence between \mathcal{Y} and \mathcal{R} . The concept of the singular-configuration-vertex-representation has been used in an *ad hoc* manner in the literature and more formally in this paper.

We can also identify a singular–configuration–vertex–representation as the set of vertices corresponding to the pivots in the rows of matrix \mathbf{M}' in the proof of Proposition 3.8. These define a vertex–representation of a fundamental system \mathcal{Y} of $\eta(G)$ distinct cores. By Proposition 3.8, deleting a vertex v in a singular–configuration–vertex–representation reduces the nullity by one and destroys a core in \mathcal{Y} that has vertex v .

Note that any collection of h vectors in B_{min} collectively cover at least h core-vertices of G . So the existence of a singular–configuration–vertex–representation is also guaranteed by *Hall's Theorem* (also known as *the Marriage Problem*).

Retaining the labelling of Proposition 3.9, there exist $\eta(G)$ singular configurations (with distinct spanning minimal configurations) which are induced subgraphs of G such that each singular configuration corresponds to a unique vertex j , $r < j \leq n$. By scaling the corresponding kernel eigenvectors so that the last non-zero entry is 1, the following result is immediate.

Corollary 3.10. *Let G be of order n and rank r , with adjacency matrix \mathbf{G} . Let the first r rows of \mathbf{G} be linearly independent vectors. There exists a matrix $\mathbf{M}^t = \begin{pmatrix} \mathbf{K} \\ \mathbf{I} \end{pmatrix}$ whose columns are the vectors of a basis for the nullspace of G , where the order of identity matrix \mathbf{I} is $n - r$.*

Note that if $\mathbf{G} = \begin{pmatrix} \mathbf{B} & \mathbf{E} \\ \mathbf{E}^t & \mathbf{U} \end{pmatrix}$ has rank r and \mathbf{B} is a non–singular $r \times r$ matrix, then $\mathbf{K} = \mathbf{B}^{-1}\mathbf{E} = -\mathbf{Y}$ in Proposition 3.9.

4 Nullity and core width

Remark 4.1. Henceforth we shall refer to a minimal basis B_{min} for $\ker(G)$ as $(\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_\eta)$. The integers $wt(\mathbf{u}_1)$ and $wt(\mathbf{u}_\eta)$ are *extremal* values and have been referred to as the graph *singularity* κ in [2, 9] and *core-width* τ in [6], respectively. We focus on the zero, non-zero pattern of the entries of the vectors in $\ker(\mathbf{G})$, to show that the nullity controls the core width.

The zero eigenvalue equation, $\mathbf{G}\mathbf{x} = \mathbf{0}$, stipulates that the sum of the entries of \mathbf{x} corresponding to neighbours of any vertex in G is zero. This is also known as the *Zero Sum Rule* [9] which leads to a generic kernel eigenvector \mathbf{x}_{gen} in terms of $\eta(G)$ independent parameters. One way in which to obtain a basis of $\eta(G)$ kernel eigenvectors is to set a parameter in turn equal to one and the remaining parameters equal to zero. If η non-zero entries of \mathbf{x}_{gen} , chosen so that they are collectively functions of all the η parameters, are set to zero, then \mathbf{x}_{gen} is forced to vanish. This concept, which has been used in the theory of singular graphs [4], will be expanded upon in this section.

The Lemma that follows appears in [1] for graphs with weighted edges. We give a new proof for the $(0 - 1)$ –adjacency matrix, emphasising the role of the core vertices in a singular graph. The result will enable us to relate the core-width τ to the nullity η , while the proof helps to shed more light on the graph structure.

Lemma 4.2. *If $\eta(G) > k \geq 1$, then there exists $\mathbf{x} \in \ker(G)$, such that \mathbf{x} has zero entries in any k specified positions.*

Proof. Let v be a core–forbidden vertex. Then any kernel eigenvector has a zero entry in that position. To prove this lemma, then, we need to show that there exists a kernel eigenvector with zeros in any k positions corresponding to core vertices.

Let the k chosen core vertices be labelled first, followed by the rest of the core vertices and ending with the core-forbidden vertices. Let \mathbf{M} be the matrix whose rows are the vectors of a basis for the nullspace of G , ordered so that the i th entry in the i th row vector is non-zero. The only non-zero entries lie in the first $|CV|$ columns. Row-reducing \mathbf{M} to echelon form, with all entries in the columns above and below a leading 1 being zero, produces a matrix \mathbf{M}' , whose rows give a new basis for the nullspace of G . Thus each row of \mathbf{M}' is non-zero. Furthermore, the pivots in the rows from the $(k + 1)$ th up to the last row have at least k zero entries preceding them. Thus the kernel eigenvectors represented by each of the last $\eta(G) - k$ rows of \mathbf{M}' satisfy the conditions of the required result. \square

Lemma 4.2 guarantees a kernel eigenvector with zero entries in any $\eta(G) - 1$ specified positions. In the proof, the rows of \mathbf{M}' form a basis that can determine the minimum weight sequence and one of a possible number of minimal bases. The determination of the minimum rank of a $(0 - 1)$ -adjacency matrix, as τ varies, is regarded as an *extremal* problem. The minimum rank for various values of τ is given in Figure 2. The result that follows holds for minimal bases.

Proposition 4.3. *If $\mathbf{x} \in B_{min}$, then \mathbf{x} has at least $\eta(G) - 1$ zero entries.*

Proof. There exists a basis B of kernel eigenvectors which are the rows of the $\eta \times n$ matrix \mathbf{M}' , with all entries in the columns above and below a pivot being zero. Recall that the set of vertices corresponding to the pivots represents a singular-configuration-vertex-representation. Thus any row of \mathbf{M}' has at least $|\eta(G)| - 1$ zero entries corresponding to all the other rows of \mathbf{M}' . By Theorem 3.2, the weight-sequence of B_{min} is entry-wise less than that of B . Thus if $\mathbf{x} \in B_{min}$, then \mathbf{x} has at least $\eta(G) - 1$ zero entries. \square

By Proposition 3.2, among all (ordered) bases for the nullspace of \mathbf{G} , a minimal basis has the maximum number of zeros in each vector in turn. The minimum number of zeros in the vectors of a minimal basis is used to establish a method of obtaining an upperbound for the nullity.

Proposition 4.4. *If the number of zero entries in a vector $\mathbf{x} \in B_{min}$ is less than k , then $\eta(G) \leq k$.*

Proof. By Proposition 4.3, all the vectors in B_{min} have $\eta - 1$ or more zero entries so that $k - 1 \geq \eta - 1$, as required. \square

Note that Proposition 4.4 can also be proved by using Lemma 4.2 directly. This guarantees a vector \mathbf{y} in the nullspace with at least k zeros if $\eta(G) > k$. So suppose that $\eta(G) > k$ and the number of zero entries in each $\mathbf{x} \in B_{min}$ is $k - 1$ or less. Since \mathbf{y} is a linear combination of the vectors in B_{min} , by Theorem 3.2, it cannot have more than $k - 1$ zero entries, contradicting the necessary condition of Lemma 4.2. Hence $\eta(G) \leq k$.

To determine the minimum number of zeros over all $\mathbf{x} \in B_{min}$, it suffices to determine the core-width τ , an invariant of the graph. Figure 2 shows all the cores of order up to six and the minimum rank of graphs with a min-max core-order (or core-width) τ .

We now show that τ and η exert mutual control.

Proposition 4.5. *For a graph G on n vertices of nullity η and core width τ , $\tau + \eta \leq n + 1$.*

Proof. By definition of core-width τ , there exists $\mathbf{y} \in B_{min}$ having τ non-zero entries. If z denotes the number of zero entries in \mathbf{y} , then $\tau + z = n$. By Proposition 4.3, $z \geq \eta(G) - 1$. Thus $\tau + \eta(G) - 1 \leq n$, as required. \square

We may ask what the threshold order of a singular graph G needs to be for a particular core F to lie in a fundamental system \mathcal{F} of cores.

Corollary 4.6. *A singular graph G of nullity η cannot have a core F_t of order t in \mathcal{F} if $t > n + 1 - \eta$.*

Definition 4.7. Let the order of a singular graph G be n . If the nullity is η and the core width is τ , then G is said to be **extremal singular** if $\eta + \tau$ reaches $n + 1$.

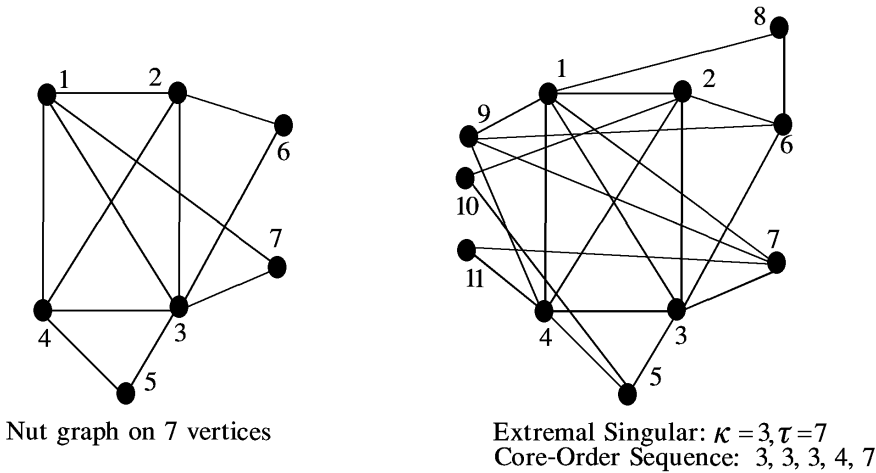


Figure 4: The nut graph 7b and a extremal singular graph of nullity five.

To determine for which graphs $\tau + \eta$ reaches the upper bound $n + 1$, we need to consider as large a core width τ as is possible, for a given core-order n and nullity η . Figure 4 shows a core graph which is extremal singular with the nut graph N_{7b} in a fundamental system of cores.

Proposition 4.8. *A graph G is extremal singular of nullity η , if and only if it is a core graph and the largest core in a fundamental system is a nut graph N and there are exactly $\eta - 1$ vertices of G not on N .*

Proof. Let $\tau + \eta = n + 1$ and $\mathbf{x} \in B_{min}$ have τ non-zero entries representing core F_τ . If z denotes the number of zero entries in \mathbf{x} , then $\tau + z = n$ and z needs to be $\eta - 1$. As in the proof of Proposition 4.3, there exists a subset L consisting of $\eta - 1$ vertices in a singular-configuration-vertex-representation representing the cores for B_{min} other than F_τ , such that at the vertex positions of L , the entries of \mathbf{x} are zero, but the entries of the other $\eta - 1$ vectors in B_{min} are collectively non-zero. Then corresponding to each vertex of G , there is a kernel eigenvector with a non-zero entry in the associated position. Hence each vertex

of G is a core vertex. Now deleting L destroys exactly $\eta - 1$ cores of G leaving a subgraph H of G of order τ with core F_τ whose kernel eigenvector has τ non-zero entries. Thus G is a core graph and H is a nut graph whose kernel eigenvector is the non-zero part of \mathbf{x} .

Conversely, if in a core graph G , the core corresponding to the core-width τ is a nut graph N , then $\tau + \eta(N) = |N| + 1$. By Proposition 3.8, as each of the $\eta - 1$ vertices is added to N to produce G , the graph proceeds through a series of core graphs. Both sides of the equation increases by one at each stage. Thus $\tau + \eta(G) = |G| + 1$. \square

Proposition 4.9. *A graph G is extremal singular of nullity one if and only if G is a nut graph.*

Proof. Recall that a nut graph is a core graph of nullity one. Thus $\tau = n$ and $\tau + \eta$ reaches the upper bound. Now for a graph with nullity one which is not a nut graph, there exist core-forbidden vertices so that $\tau < n$. \square

Thus a nut graph of order n_1 is extremal singular and may be grown into larger extremal singular graphs with core width n_1 .

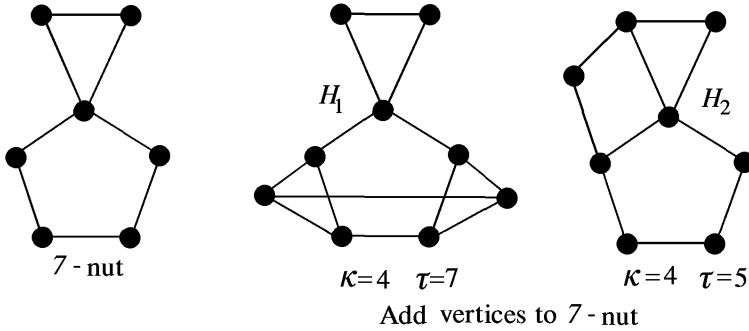


Figure 5: Non-extremal core graphs H_1 and H_2 of nullity two - with the nut graph N_{7a} as an induced subgraph.

When starting from a nut graph (N, \mathbf{x}_N) , to construct a singular graph of nullity η , in such a way that the nullity increases with each vertex addition, the vector \mathbf{x}_N need not remain in a minimal basis. Indeed, let us start with a nut graph N and add vertices to produce a core graph. If with each vertex added, a core graph is created while (N, \mathbf{x}_N) is preserved, then the nullity increases by one with each vertex addition and the equality $|N| + \eta(G) = n + 1$ holds. If the core-width $\tau(G) = |N|$, then G is extremal singular. However, there are two other possibilities that might occur in the process of vertex addition until the n -vertex core graph G is produced. With some vertex addition, either a core is not created or the core (N, \mathbf{x}_N) is not preserved in a basis B_{min} for the enlarged graph G . In the former case the nullity does not reach the maximum possible for n and τ , whereas in the latter case \mathbf{x}_N does not remain the non-zero part of a vector in a basis B_{min} for the nullspace of the adjacency matrix of the enlarged graph obtained. If either of these cases occurs, even though the nut graph N remains an induced subgraph and \mathbf{x}_N is still a kernel eigenvector of the enlarged graph, $\tau + \eta < n + 1$, and the core graph obtained is not extremal singular. The graphs in Figure 5 illustrate these two cases. The nine-vertex

graph H_1 has $\kappa = 4$ and $\tau = 7$, with F_τ being the nut graph N_{7a} (the smallest nut graph possible [10]). The nullity is two, however, not three as required for $\tau + \eta = n + 1$, because the nullity did not increase on adding the first vertex to the nut graph N_{7a} . Note that the eight vertex graph H_2 , in Figure 5, has nullity two as well. Although the nut graph N_{7a} is an induced subgraph and a core of H_2 , τ is not preserved. Thus the nut graph N_{7a} fails to remain in a Fundamental System of cores (determined by a $B_{min}(H_2)$) after the eighth vertex is added.

Proposition 4.10. *Let G be a singular graph of nullity η , having a fundamental system \mathcal{F} of cores. Then $\max_{F \in \mathcal{F}} (|F| + \eta(F)) + \eta(G) \leq n + 2$.*

Proof. Let $F \in \mathcal{F}$ have kernel eigenvector \mathbf{x}_F . By Proposition 3.7, there exists a singular configuration H of order $|F| + \eta(F) - 1$ with core (F, \mathbf{x}_F) as an induced subgraph of G . By interlacing, G has at least $|H| + \eta(G) - 1$ vertices. Hence $n \geq |F| + \eta(F) + \eta(G) - 2$ for all $F \in \mathcal{F}$. □

A core in a fundamental system may be a nut graph in which case it is both a core of G and an induced singular configuration of G . If G is extremal singular, then by Proposition 4.8, a core of maximum order τ in \mathcal{F} is a nut graph. Recall that any core F , in a fundamental system \mathcal{F} of cores of a graph G is an induced subgraph of a singular configuration H which is in turn an induced subgraph of G . Now by definition, $|F| \leq \tau$ but is $|H| \leq \tau$? This is extremely pertinent when a core in a fundamental system \mathcal{F} of cores of a graph G is rK_1 . In this case, the order, $2|F| - 1$, of H is relatively large when compared to $|F|$, in contrast with the case when F is a nut graph and $|H| = |F|$.

Lemma 4.11. *Let G be an extremal singular graph with core width τ and nullity η . Let F be a core in a fundamental system of cores of G . Then $\tau \geq |F| + \eta(F) - 1$.*

Proof. Since G is extremal singular, $\eta(G) + \tau = n + 1$. By Proposition 4.10, $|F| + \eta(F) - 1 \leq n + 1 - \eta(G) = \tau$. □

Proposition 4.12. *Let G be an extremal singular graph of nullity η and core-width τ . Let F be a core having a fundamental system \mathcal{F} of cores. If H is an induced subgraph of G which is a singular configuration with core F , then $|H| \leq \tau$.*

Proof. Let H be a singular configuration which is an induced subgraph of G corresponding to the core F . By Lemma 4.11, $|H| = |F| + \eta(F) - 1 \leq \tau$. □

Example 4.13. The singular configurations of the extremal singular graph of Figure 4, associated with the cores $3K_1, 3K_1, 3K_1, C_4$, and the nut graph N_{7a} in a fundamental system, have order 5, 5, 5, 5, 7 respectively, supporting Proposition 4.12.

The graphs H_1 and H_2 of Figure 5 are not extremal singular. The graph H_1 has core-order sequence $\{4, 7\}$ corresponding to cores C_4 and the nut graph N_{7a} , associated to singular configurations of order 5 and 7 respectively. The graph H_2 has core-order sequence $\{4, 5\}$ corresponding to cores $4K_1$ and $C_4 \dot{\cup} K_1$, associated to singular configurations of order 5 and 7 respectively.

Corollary 4.14. *If core rK_1 is in fundamental system of cores of an extremal singular graph, then $r \leq \lfloor \frac{\tau}{2} \rfloor$.*

Proof. A singular configuration H with core rK_1 has $(2r-1)$ vertices. Then $|H| = 2r-1$. By Proposition 4.12, $|H| \leq \tau$. Hence the integer $r \leq \frac{\tau+1}{2}$. \square

5 Conclusion

The symmetry of the $(0-1)$ -adjacency matrix \mathbf{G} of rank r enables its representation as a block matrix with a maximally non-singular $(r \times r)$ -principal submatrix of \mathbf{G} . The nullspace of \mathbf{G} can be expressed in terms of submatrices of this representation.

The presence of singular configurations as induced subgraphs in a graph is a necessary condition for a graph to be singular. In a graph G of nullity η , we showed that there is a vertex representation \mathcal{R} consisting of η vertices corresponding to η singular configurations which are induced subgraphs of G . The choice of the vertices in \mathcal{R} , which are core vertices, is not unique. A graph may have core-forbidden vertices that do not lie on any core of G . Deletion of a core-forbidden vertex either increases the nullity or leaves it unchanged.

The core-width τ (maximum weight of the vectors in a minimal basis for the nullspace of G) is an invariant of G and was shown to have extremal properties tied with the nullity η in a n -vertex graph. Among all graphs on n vertices, $\tau + \eta$ reaches a maximum in extremal singular graphs. Not only are the core-orders in a fundamental system \mathcal{F} of cores bounded above by τ but in extremal singular graphs, the orders of the singular configurations corresponding to the cores of \mathcal{F} are also bounded above by τ .

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